USACM Thematic Conference on

Recent Advances in Computational Methods for Nanoscale Phenomena

University of Michigan, Ann Arbor

August 29-31, 2016

Organizers:

Vikram Gavini, *University of Michigan*
Dennis Kochmann, *California Institute of Technology*
Gregory Wagner, *Northwestern University*
Jonathan Zimmerman, *Sandia National Laboratories*

The travel awards have been made possible through NSF Award CMMI-1254424 (Mechanics of Materials program), which is gratefully acknowledged.

Recent Advances in Computational Methods for Nanoscale Phenomena

GG Brown Building, Room 2505

Monday, August 29

8:00 am Registration/Light Breakfast

Session 1: 8:30 am - 10:15 am
Phase Field Models

8:30 am - 9:05 am Dayal, K., Agrawal, V., *Nucleation and Kinetics in Phase-Field Models of Twinning and Fracture*

9:05 am - 9:40 am Hunter, A., Zeng, Y., Beyerlein, I., Kozlowski, M., *Slip Transmission in FCC/FCC Bilayers using Phase Field Dislocation Dynamics (PFDD)*

9:40 am - 10:15 am Thornton, K., *Phase-Field Crystal Models: Recent Advances and Applications*

10:15 am - 10:35 am Coffee Break

Session 2: 10:35 am - 12:20 pm
Defect Mechanics I

10:35 am - 11:10 am Acharya, A., Zhang, C., Zhang, X., *Line Defect Dynamics and Solid Mechanics*

11:10 am - 11:45 am Aubrey, S., Arsenlis, A. *Anisotropic Elasticity in Dislocation Dynamics*

11:45 am - 12:20 pm Garikipati, K., Wang, Z., Rudraraju, S., *A Three Dimensional Field Formulation, and Isogeometric Solutions to Point and Line Defects using Toupin's Theory of Gradient Elasticity*

12:20 pm - 1:30 pm Lunch

Session 3: 1:30 pm - 3:15 pm
Defect Mechanics II

1:30 pm - 2:05 pm Svendsen, B., Rezaeimianroodi, J., *Atomistic and Continuum Modelling of Nanoscopic Dislocation Processes*

2:05 pm - 2:40 pm El-Azab, A., Xia, S., *Dislocation Patterns in Defored Crystals*

2:40 pm - 3:15 pm Swinburne, T., Dudarev, S., *Using Zwanzig's Technique to Investigate Stochastic Defect Dynamics*

3:15 pm - 3:35 pm Coffee Break

Session 4: 3:35 pm - 5:20 pm
From Atomistics to Larger Cells

3:35 pm - 4:10 pm Perez, D., Voter, A., *Long-Time Atomistic Simulations with Parallel Trajectory Splicing*

4:10 pm - 4:45 pm Mendez, J., Ortiz, M. *Long-term Atomistic Simulation of Diffusion: Application to Silicon-based Lithium Batteries*

4:45 pm - 5:20 pm Jones, R., Criscenti, L., *Assessing the Fracture Strength of Geological and Related Materials via an Atomistically Based J-Integral*

7:00 pm Dinner at Gandy Dancer Restaurant, 401 Depot St., Ann Arbor

Tuesday, August 30

Session 5: 8:30 am - 10:15 am
First Principles I

8:30 am - 9:05 am	Suryanarayana, P.,*Towards large and fast Density Functional Theory Calculations*
9:05 am - 9:40 am	Banerjee, A., Suryanaryana, P., *Cyclic Density Functional Theory: A Route to the First Principles Simulation of Bending in Nanostructures*
9:40 am - 10:15 am	Sukumar, N., Pask, J., *Partition of Unity Finite Element Method for Kohn-Sham Density Functional Calculations*
10:15 am - 10:35 am	Coffee Break

Session 6: 10:35 am - 11:45 am
First Principles II

10:35 am - 11:10 am	Pask, J., *Accurate Quantum Molecular Dynamics with Thousands of Atoms*
11:10 am - 11:45 am	Ghazisaeidi, M., Buey, D., Hector, L., *First Principles Modeling of <c+a> Dislocation Geometry and Interactions with Solutes in Mg Alloys*
11:45 am - 1:15 pm	Lunch

Session 7: 1:15 pm – 2:25 pm
First Principles III

1:15 pm - 1:50 pm	Yang, C., Banerjee, A., Lin, L., Hu, W., *Fast Electronic Structure Calculation Methods for Studying Low-Dimensional Nanomaterials*
1:50 pm - 2:25 pm	Lin, L., *Adaptively Compressed Exchange Operator*
2:25 pm - 3:00 pm	Coffee Break

Session 8: 3:00 pm – 4:45 pm
Coarse-Grained Atomistics

3:00 pm – 3:35 pm	Voter, A., Zamora, R., Perez, D., *Speculatively Parallelized Temperature Accelerated Dynamics*
3:35 pm – 4:10 pm	Kim, W., *Accelerated Multiscale Simulation of Nanoindentation Using Hyper-Quasicontinuum Method*
4:10 pm – 4:45 pm	Keten, S., *Coarse-grained Modeling of Nanoconfinement in Structural Nanocomposites*

Poster Session

5:00 pm - 6:30 pm	Poster Session in Lobby

Wednesday, August 31

Session 9: 8:30 am - 10:15 am
Scale-Bridging Methods

8:30 am - 9:05 am	Trinkle, D., *Bridging timescales: Automating Diffusivity Calculations for Interstitial and Solute Diffusion from First-Principles*
9:05 am - 9:40 am	Reina, C., Liu, C., *Multiscale Simulations of Wave Propagation in Heterogenous Media*
9:40 am - 10:15 am	Knap, J., Leiter, K., Barnes, B., Becker, R., Sokolow, A., Crone, J., Borodin, O., *Multiscale Computation for Materials Modeling*
10:15 am - 10:35 am	Coffee Break

Session 10: 10:35 am - 12:20pm
Metal Plasticity

10:35 am - 11:10 am	Koslowski, M., Cao, L., *Strain Rate, Grain Size Distribution and Avalanche Behavior in Nanocrystaline Metals*
11:10 am - 11:45 am	Marian, J., Cereceda, D., Diehl, M., Roters, F., Raabe, D., *Predicting the Temperature Dependence of the Yield Strength in BCC Metals using Atomistically-Informed Crysta Plasticity Calculation*
11:45 am -12:20 pm	Spearot, D., Aksoy, D., Barrows, W., Dingreville, R., *Decohesion Relationships for Grain Boundary Fracture in Nickel extracted from Molecular Dynamics Simulations*
12:20 pm -1:30 pm	Lunch

Session 11: 1:30-3:15pm
Mechanics of Materials

1:30 pm - 2:05 pm	Woodward, C., Rao, S., Hussein, A., Akdim, B., Antillon, E., Dimiduk, D., *Intrinsic Scale Effects in Metal Deformation*
2:05 pm - 2:40 pm	Tucker, G., *Resolving the Correlation between Microstructure and Nanoscale Deformation Mechanisms in Metallic Nanostructured Materials*

Posters

(listed alphabetically by presenter)

Nikhil Chandra Admal, *A Thermodynamically Consistent Diffuse Interface Crystal Plasticity Model to Study Grain Growth During Dynamic Recrystallization*

Vinamra Agrawal, *Shock Induced Phase Transition in Ferroelectric Materials*

Andrew Binder, *A Predictor-Corrector Method for Efficient Modeling of Surface Effects*

Subhendu Chakraborty, *Near-Crack Phenomenon Modelling Using Finite Temperature Coupled Atomistic-Continuum Self-Consistent Method*

Sambit Das, *Application of Real Space Density Functional Theory to Dislocation Studies in Al and Mg*

Arnab Debnath, *Solving Boltzmann Equation using Finite Element Methods for Affine and Viscometric Flows*

Swarnava Ghosh, *SPARC: A Framework for Efficient Large-Scale Real Space Density Functional Theory Calculations*

Bikash Kanugo, *Large-scale All-electron Density Functional Theory Calculations using Enriched Finite Element Method*

Juan P. Mendez Granado, *Stable Grain Boundary Structures in Graphene*

Phani Motamarri, *Real Space Finite-Element Based Large-Scale Electronic-Structure Calculations: A Route to High Fidelity Description of Material Properties*

Brandon Runnels, *Modeling Grain Boundary-Driven Microstructural Evolution with an Analytical Model for Grain Boundary Anisotropy and the Phase Field Method*

William J. Schill, *A Spectral Discretization Scheme for Density Functional Theory*

Soumya Mukherjee, *Electron Scattering in Periodic and Symmetry Adopted Structures with Defect*

Dingyi Sun, *The Twinning Genome: A Systematic Framework for Predicting Twinning in Materials*

Ishan Tembhekar, *Fully-Nonlocal 3D Quasicontinuum Modeling of Defect Interactions with Grain Boundaries*

Haoran Wang, *Design of Robust Solid-Electrolyte Interphase in Li-ion Battery by Multiscale Simulations*

Xin Wang, *Lanczos-Based Approaches to Solving the Kohn-Sham Equations*

Xingjie Li, *Blended-Force Based Quasicontinuum Method for Multilattices Crystals*

Qimen Xu, *Helical Density Functional Theory: A Route to the First Principles Simulation of Torsion in Nano-Structures*

Qingcheng Yang, *Multiresolution Molecular Mechanics: A Generalized Nonlocal Quasicontinuum Framework*

Zhong Zhou, *Multiphysics Simulation of Meniscus-Confined Electrodeposition Based 3D-Nanoprinting*

Abstracts

Monday, August 29, Session 1: 8:30-9:05
Phase Field Models
Nucleation and Kinetics in Phase-Field Models of Twinning and Fracture
Kaushik Dayal, Vaibhav Agrawal, *Carnegie Mellon University*

Phase-field models enable easy computations of microstructure because they regularize sharp interfaces and cracks. In addition, the nucleation of new interfaces and the kinetics of existing interfaces occurs "automatically" using only the energy and a gradient descent dynamics. This automatic nucleation and kinetics is often cited as an advantage of these models, and is not present in sharp interface approaches where nucleation and kinetics must be explicitly prescribed. However, this is not necessarily an advantage. Rather, it does not allow us to use nucleation and kinetic insights that may be gained from experiment and/or molecular simulations. Hence, this feature is actually a disadvantage because it breaks the multiscale modeling hierarchy of feeding information through the scales. Motivated by this, we have developed a phase-field model (i.e., with regularized interfaces) that allows for easy and transparent prescription of kinetics and nucleation. We present the formulation of the model, and characterization through various examples in applications to fracture and structural transformations such as twinning.

Monday, August 29, Session 1: 9:05-9:40
Phase Field Models
Slip Transmission in FCC/FCC Bilayers using Phase Field Dislocation Dynamics (PFDD)
Abigail Hunter[1], Yifei Zheng[2], Irene J. Beyerlein[3], Marisol Kozlowski[2],
[1]Los Alamos Laboratory, [2]Purdue University, [3]University of California at Santa Barbara

This research presents the formulation of a phase field dislocation dynamics model designed to treat a system comprised of two materials differing in moduli and lattice parameters, meeting at a common interface. We use it to investigate the critical stress required to transmit a perfect dislocation across a bimaterial interface with a cube-on-cube orientation relationship. The calculation of the critical stress accounts for the effects of: 1) the stresses induced at the interface due to the lattice mismatch (misfit or coherency stresses), 2) the elastic moduli mismatch (Koehler forces or image stresses) and 3) the formation of the residual dislocation. Our results show that the critical stress associated with the transmission of a dislocation from material 1 to 2 is not the same as from material 2 to 1. We find that the transmission from the material with the lower shear modulus is easier than the reverse and the degree of asymmetry in critical stress is directly proportional with the lattice mismatch. An analytical model for the critical stress is also presented. It is based on the formation energy of the residual dislocation and shows good comparison with the simulated results in the limit of large mismatch for coherent interfaces. The analytical model predicts a scaling factor for the critical stress that is based on the shear moduli and lattice parameters of both materials that will also be discussed.

Monday, August 29, Session 1: 9:40-10:15
Phase Field Models
Phase-Field Crystal Models: Recent Advances and Applications
Katsuyo Thornton, *University of Michigan*

The phase-field crystal (PFC) model describes the evolution of atomic positions via a partial differential equation for a continuous field. It can be applied to study a wide variety of material processes such as nucleation, phase transformation, solid-liquid interfacial energetics, and dislocation and grain boundary dynamics. PFC is emerging as a promising tool for predicting material properties and behavior because it retains atomic resolution while accessing the diffusive time scale. As such, the PFC model acts as a bridge between atomistic models and

mesoscale models. However, much work is still needed in order to generate quantitative predictions using the approach. After an overview of the PFC model and our past work, we will discuss a few of our recent works on PFC: (1) equilibrium grain boundary structures and predicted energies, with a comparison with molecular dynamics results, and (2) a PFC model for two-dimensional materials.

Monday, August 29, Session 2: 10:35-11:10
Defect Mechanics I
Line Defect Dynamics and Solid Mechanics
Amit Acharya[1], Chiqun Zhang[1], Xiaohan Zhang[2]
[1]*Carnegie Mellon University*, [2]*Stanford University*
Continuum mechanics has been a successful model for studying macroscopic deformations and the forces causing them. The usual framework allows the study of continuous deformations giving way to surfaces of discontinuity, but does not provide an adequate framework for considering the dynamics of the terminating lines of surfaces of discontinuity, were such to occur. It turns out that such terminating lines of surfaces of discontinuity serve as a model of common line defects that arise in a host of materials; dislocations and grain/phase boundary junctions in crystalline and soft matter. I will describe a framework for considering line defect dynamics within continuum mechanics. I will show how the kinematics of line defect dynamics provides a unifying theme for describing the defects mentioned above, resulting in an augmentation of the classical balance laws of continuum mechanics with a microscopic conservation law for topological charge carried by these defect lines. The theory will be illustrated with examples related to dislocation dynamics with inertia, the computation of fields of interfacial defects like the star disclination and grain boundary disconnections.

Monday, August 29, Session 2: 11:10-11:45
Defect Mechanics I
Anisotropic Elasticity in Dislocation Dynamics
Sylvie Aubry, Athanasios Arsenlis, *Lawrence Livermore National Laboratory*
Dislocation dynamics simulations often assume isotropic elasticity to compute stresses at points in the simulation volume and forces between dislocations. Anisotropic elasticity has been used to compute dislocation reactions and dynamics for small dislocation ensembles such as a dislocation loop, a Frank–Read source and two straight, interacting dislocations. For large, dense dislocation ensembles, anisotropic elasticity is rarely used due to its perceived computational cost. Most large-scale simulations have resorted to using isotropic elastic approximations that are less computationally intensive. Large-scale dislocation dynamics simulations usually involve several millions of interacting dislocation segments. The stress at a point and interaction force between two dislocation segments need to be computed many times during simulations. We evaluate the cost versus accuracy of evaluating the interaction force between dislocation lines using the direct and the fast multipole methods and present large-scale simulations illustrating the use of anisotropic elasticity in dislocation dynamics simulations.

Monday, August 29, Session 2: 11:45-12:20
Defect Mechanics I
A Three Dimensional Field Formulation, and Isogeometric Solutions to Point and Line Defects using Toupin's Theory of Gradient Elasticity
Krishna Garikipati, Zhenlin Wang, Shiva Rudraraju, *University of Michigan*
We present a field formulation for defects that draws from the classical representation of the cores as force dipoles. We write these dipoles as singular distributions. Exploiting the key insight that the variational setting is the only appropriate one for the theory of distributions, we arrive at universally applicable weak forms for defects in nonlinear elasticity. Remarkably, the standard, Galerkin finite element method yields numerical solutions for the elastic fields of defects that, when parameterized suitably, match very well with classical, linearized elasticity solutions. The true potential of our approach, however, lies in its easy extension to generate solutions to elastic fields of defects in the regime of nonlinear elasticity, and even more notably for Toupin's theory of gradient elasticity at finite strains (Arch. Rat. Mech. Anal., 11, 385, 1962).

In computing these solutions we adopt recent numerical work on an isogeometric analytic framework that enabled the first three-dimensional solutions to general boundary value problems of Toupin's theory (Rudraraju et al. Comp. Meth. App. Mech. Engr., 278, 705, 2014). We first present exhaustive solutions to point defects, edge and screw dislocations, and a study on the energetics of interacting dislocations. Then, to demonstrate the generality and potential of our treatment, we apply it to other complex dislocation configurations, including loops and low-angle grain boundaries.

Monday, August 29, Session 3: 1:30-2:05
Defect Mechanics II
Atomistic and Continuum Modelling of Nanoscopic Dislocation Processes
Bob Svendsen, Jaber Rezaeimianroodi, *RWTH Aachen University*

The purpose of this work is the development of continuum models for dislocation-mediated processes in nanocrystals. In particular, this is based on a detailed theoretical and computational comparison of such models with each other as well as with atomistic modeling based on molecular statics (MS) and molecular dynamics (MD). Continuum models compared theoretically in the current work include field dislocation mechanics (FDM: e.g., Acharya, JMPS 58, 766-778, 2010; Gbemou et al., Int. J. Plast. 82, 241-259, 2016), generalized Peierls-Nabarro (GPN: e.g., Xiang et al., Acta Mat. 56, 1447-1460, 2008), phase-field dislocation dynamics (PFDD: e.g., Hunter et al., Phys. Rev. B 84, 144108, 2011), atomistic phase-field microelasticity (APFM; Mianroodi, Svendsen, JMPS 77, 109- 122, 2015), and phase field crystal (PFC: e.g., Berry et al., Phys. Rev. B 86, 224112, 2012; B 89, 214117, 2014). In contrast to MS and MD, which are geometrically non-linear, all of these are geometrically linear models. The recent extension of APFM to geometric non-linearity (Mianroodi, Svendsen, submitted, 2016) will also be discussed. Comparison of continuum and atomistic results is based in particular on the unification of disregistry-based (continuum) and coordination-based (atomic) detection of dislocation lines (cores), stacking faults, and lattice states such as “unslipped”, “slipped”, “twinned”, or “restacked”. Computational comparisons of GPN, PFDD, APFM (geometrically linear- and non-linear), MS and MD are carried out in the context of the simulation of elementary dislocation processes such as dissociation, core and stacking fault formation, glide, or cross slip.

Monday, August 29, Session 3: 2:05-2:40
Defect Mechanics II
Dislocation Patterns in Deformed Crystals
Anter El-Azab, Shengxu Xia, *Purdue University*

A theoretical-computational continuum dislocation dynamics framework of crystal plasticity will be presented. This framework has two components. The first is a density-based formulation of dislocation motion and interactions fully coupled with crystal mechanics, and the second is a time coarse graining procedure for the rate processes that enables us to inform the density-based formulation using discrete dislocation dynamics. A lattice-inspired finite element methods has been developed to solve the overall model equations. Self-organized dislocation patterns agreeing with experimental observations under both monotonic and cyclic loading have been successfully predicted. The results show the emergence of cell structure formation in fcc crystal under [001] loading and the morphing of this structure into lamellar structure under [011] and [111] type loading. The similitude law for the average cell size evolution as the inverse of stress is demonstrated. Cross slip was found to be critical for triggering the dislocation patterning process in the case of monotonic loading. The famous vein structure was also predicted under cyclic loading; it was observed that the self-organization of dislocations on individual slip systems resembles that observed under single slip loading. After articulating the theory and computational and presenting the key results, the presentation will end with a perspective on connecting the current modeling approach with TEM and X-ray measurements and the modeling of recrystallization in metals.

Monday, August 29, Session 3: 2:40-3:15
Defect Mechanics II
Using Zwanzig's Technique to Investigate Stochastic Defect Dynamics
Thomas D. Swinburne, Sergei L. Dudarev, *Culham Centre for Fusion Energy*
Stochastic thermal forces play a crucial role in the dynamics of point defects and dislocations. When the migration barrier is low, thermal forces give rise to the viscous phonon drag, whilst large barriers are crossed by thermal activation. I will talk about theoretical and numerical techniques developed to capture the forces on crystal defects directly from the atomic forces using Zwanzig's projection technique, resolving long-standing anomalies in phonon drag theory and allowing access to new statistical techniques to analyze defect dynamics.

Monday, August 29, Session 4: 3:35-4:10
From Atomistics to Larger Cells
Long-Time Atomistic Simulations with the Parallel Trajectory Splicing
Daniel Perez, Arthur Voter, *Los Alamos National Laboratory*
Molecular Dynamics (MD) is a workhorse of computational materials science. Indeed, MD can in principle be used to obtain any thermodynamic or kinetic quantity, without introducing approximation or assumptions beyond the adequacy of the interaction potential. This enviable quality however comes at a steep computational price, hence limiting the system sizes and simulation times that can be achieved in practice. While the size limitation can be efficiently addressed with massively parallel implementations of MD based on spatial decomposition strategies, the same approach usually cannot extend the timescales much beyond microseconds. In this talk, we discuss a novel approach, Parallel Trajectory Splicing (ParSplice) that aims at addressing the timescale limitation of MD for systems that evolve through rare state-to-state transitions. As with the Parallel Replica Dynamics method, the problem is instead parallelized in the time domain. The key innovation of ParSplice lies in the use of speculation on the future evolution of the dynamical trajectory in order to expose additional parallelism by allowing work to simultaneously proceed in many states. This is achieved through a concurrent stochastic simulation parameterized on the fly. We review the formal underpinnings of the method and demonstrate that it can provide arbitrarily accurate results for any definition of the states while providing significant improvement in computational efficiency compared to its predecessors. We then demonstrate the usefulness of ParSplice by presenting different examples of materials simulations where access to long timescales was essential to access the physical regime of interest.

Monday, August 29, Session 4: 4:10-4:45
From Atomistics to Larger Cells
Long-Term Atomistic Simulation of Lithiation in Silicon-Based Lithium Batteries
J.P. Mendez[1], M. Ponga[2], M. Ortiz[2]
[1]California Institute of Technology, [2]The University of British Columbia
Lithiation is a fundamental process that takes place in Si anodes in Li batteries when lithium cations enter the Si lattice during electric charge. Upon lithiation, Si anodes loses its crystalline structure and the alloy becomes amorphous, with a considerable volume increase. This, in turn, creates large internal stresses that may induce plastic deformation, damage and fracture of the Si anode.

Monday, August 29, Session 4: 4:45-5:20
From Atomistics to Larger Cells
Assessing the Fracture Strength of Geological and Related Materials via an Atomistically Based J-Integral
Reese Jones, Louise Criscenti, *Sandia National Laboratories*

Predicting fracture initiation and propagation in low-permeability geomaterials is a critical yet un- solved problem crucial to assessing shale caprocks at carbon dioxide sequestration sites, and controlling fracturing for gas and oil extraction. Experiments indicate that chemical reactions at fluid-geomaterial interfaces play a major role in subcritical crack growth by weakening the material and altering crack nucleation and growth rates. Engineering the subsurface fracture environment, however, has been hindered by a lack of understanding of the mechanisms relating chemical environment to mechanical outcome, and a lack of capability directly linking atomistic insight to macroscale observables.

We have developed a fundamental atomic-level understanding of the chemical-mechanical mechanisms that control subcritical cracks through coarse-graining data from reactive molecular simulations. Previous studies of fracture at the atomic level have typically been limited to producing stress-strain curves, quantifying either the system-level stress or energy at which fracture propagation occurs. As such, these curves are neither characteristic of nor insightful regarding fracture features local to the crack tip. In contrast, configurational forces, such as the J-integral, are specific to the crack in that they measure the energy available to move the crack and truly quantify fracture resistance. By development and use of field estimators consistent with the continuum conservation properties we are able to connect the data produced by atomistic simulation to the continuum-level theory of fracture mechanics and thus inform engineering decisions. In order to trust this connection we have performed theoretical consistency tests and validation with experimental data. Although we have targeted geomaterials, this capability can have direct impact on other unsolved technological problems such as predicting the corrosion and embrittlement of metals and ceramics.

Tuesday, August 30, Session 5: 8:30-9:05
First Principles I
Towards Large and Fast Density Functional Theory Calculations
Phanish Suryanarayana, *Georgia Institute of Technology*

Electronic structure calculations based on Density Functional Theory (DFT) have been remarkably successful in describing material properties and behavior. However, the large computational cost associated with these simulations has severely restricted the size of systems that can be routinely studied. In this talk, previous and current efforts of the speaker to develop efficient real-space formulations and parallel implementations for DFT will be discussed. These include linear scaling methods applicable to both insulating and metallic systems.

Tuesday, August 30, Session 5: 9:05-9:40
First Principles I
Cyclic Density Functional Theory: A Route to the First Principles Simulation of Bending in Nanostructures
Amartya Banerjee[1], Phanish Suryanaryana[2]
[1]*Lawrence Berkeley National Laboratory*, [2]*Georgia Institute of Technology*

We formulate and implement Cyclic Density Functional Theory (Cyclic DFT) -- a self-consistent first principles simulation method for nanostructures with cyclic symmetries. Using arguments based on Group Representation Theory, we rigorously demonstrate that the Kohn-Sham eigenvalue problem for such systems can be reduced to a fundamental domain (or cyclic unit cell) augmented with cyclic-Bloch boundary conditions. Analogously, the equations of electrostatics appearing in Kohn-Sham theory can be reduced to the fundamental domain augmented with cyclic boundary conditions. By making use of this symmetry cell reduction, we show that the ground-state energy and the Hellmann-Feynman forces on the atoms can be calculated using quantities defined over the fundamental domain. In order to have a fully functional numerical realization of the proposed approach, we investigate possible discretization strategies-- including a symmetry adapted spectral scheme as well as a scheme based on finite-

differences. In particular, we follow up on our finite difference discretization scheme and demonstrate through selected examples that our formulation and implementation of Cyclic DFT is both accurate and efficient.

The connection of cyclic symmetries with uniform bending deformations provides an elegant route to the ab-initio study of bending in nanostructures using Cyclic DFT. As a demonstration of this capability, we simulate the uniform bending of a silicene nanoribbon and obtain its energy-curvature relationship from first principles. A self-consistent ab-initio simulation of this nature is unprecedented and well outside the scope of any other systematic first principles method in existence. We describe several future avenues and applications of Cyclic DFT, including its extension to the study of non-uniform bending deformations and its possible use in the study of the nanoscale flexoelectric effect.

Tuesday, August 30, Session 5: 9:40-10:15
First Principles I
Partition of Unity Finite Element Method for Kohn-Sham Density Functional Calculations
N. Sukumar[1], John Pask[2]
[1]*University of California, Davis,* [2]*Lawrence Livermore National Laboratory*

The current state-of-the-art for large-scale quantum-mechanical simulations is the planewave (PW) pseudopotential method, as implemented in codes such as VASP, ABINIT, QBox, and many others. However, since the PW method uses a global Fourier basis, with strictly uniform resolution at all points in space, it suffers from substantial inefficiencies in calculations involving atoms with localized states, such as first-row and transition-metal atoms, and requires significant nonlocal communications that compromises parallel efficiency. Real-space methods such as adaptive finite-differences and finite-elements have partially addressed both resolution and parallel-communications problems, but have been plagued by one key disadvantage relative to PW: excessive number of degrees of freedom (basis functions) needed to achieve the required accuracies. In this talk, I will present a real-space partition of unity finite element (PUFE) approach to solve the Kohn-Sham equations (coupled Schrodinger and Poisson equations) of density functional theory. In the PUFE method, we build the known atomic physics into the solution process to solve the Schrodinger eigenproblem using partition-of-unity enrichment techniques in finite element analysis. The method developed herein is completely general, applicable to any crystal symmetry and to both metals and insulators alike. Total energy calculations for full self-consistent Kohn-Sham calculations will be presented for LiH that has light atoms, as well as triclinic CeAl (f-electron system), which requires large numbers of atomic-orbital enrichments. Numerical issues such as efficient numerical integration and ill-conditioning of the basis set will be discussed. The new PUFE approach attains the required accuracies with substantially fewer degrees of freedom, typically by an order of magnitude or more, than the PW method. We also perform an equation of state calculation for LiH and show that the computed lattice constant and bulk modulus from first principles is in agreement with reference results.

Tuesday, August 30, Session 6: 10:35-11:10
First Principles II
Accurate Quantum Molecular Dynamics with Thousands of Atoms
John Pask, *Lawrence Livermore National Laboratory*

Quantum molecular dynamics (QMD) simulations occupy a significant fraction of supercomputer resources around the world every day. The method of choice in the vast majority of such simulations has been the planewave method, as implemented in VASP, ABINIT, and many others. However, due to the extreme demands of such simulations, requiring the solution of the Kohn-Sham equations in at most a few minutes, tens or hundreds of thousands of times over, the size of systems which can be investigated by such accurate means has been severely limited, typically to a few hundred atoms or less. In this talk, we discuss our work on new electronic structure methodology to push back these limits, allowing full Kohn-Sham simulations of systems containing thousands of atoms, thus opening the way to model a range of systems previously accessible only to more approximate, empirical methods. The key points of departure making this possible are (1) the use a discontinuous basis, and (2) the elimination of

diagonalization, while retaining strict systematic improvability, and applicability to metals and insulators alike. We discuss the path from classical finite elements to enriched finite elements to discontinuous Galerkin methods as we now employ, as well as two particularly efficient options for obtaining densities, energies, and atomic forces from the discrete Hamiltonian, once constructed. We highlight applications of the new methodology to anode-electrolyte interface simulations in lithium-ion battery systems, and note outstanding issues to be confronted in order to move from 5,000 to 10,000 atoms and more.

Tuesday, August 30, Session 6: 11:10-11:45
First Principles II
First Principles Modeling of <c+a> Dislocation Geometry and Interactions with Solutes in Mg Alloys
Maryam Ghazisaeidi[1], Daniel Buey[1], Lou Hector[2]
[1]Ohio State University, [2]General Motors R&D
Predicting mechanical properties of new alloys requires understanding the atomic-scale mechanisms of plasticity with an accurate account for chemistry change. First principles modeling of dislocation core structures and interactions with solutes, is a fundamental step towards quantitative and predictive design of new alloys for enhanced and tailored properties. For example, activation of the pyramidal <c+a> slip mode—with an order of magnitude higher critical stress than the basal slip mode-- enhances room temperature ductility of Mg alloys. We compute the core structure and energy of edge and screw <c+a> dislocations using density functional theory (DFT) in combination with lattice Green's function boundary conditions. Both dislocations dissociate into two half <c+a> partials separated by a stacking fault on the (1-212) plane. The edge dislocation pyramidal II core structure is then used to study the effect of Y solutes at several positions inside the dislocation core. The presence of Y in several of these sites modifies the core structure as follows. When placed inside the partial dislocation cores, Y severely distorts the surrounding bonds. On the other hand when Y is put on the stacking fault region, separating the partials, the dissociation distance can change by about the magnitude of the <c+a> Burgers vector, often accompanied by lowering the energy. We then used a modified Labusch-type solid solution strengthening model to predict the stress required to move the dislocation in the presence of Y from first-principles interaction energies.

Tuesday, August 30, Session 7: 1:15-1:50
First Principles III
Fast Electronic Structure Calculation Methods for Studying Low-Dimensional Nanomaterials
Chao Yang, Amartya Banerjee, Lin Lin, Wei Hu, *Lawrence Berkeley National Laboratory*
Low-dimensional materials such as graphene and phosphorene nanoribbons and nanoflakes exhibit intriguing phenomena. Their electronic properties depend on how they are cut from bulk materials, i.e., their edge types, how edges are passivated, the presence of defects, and their sizes. Efficient and reliable computational tools must be used to study these nanomaterials, which can contain more than 10,000 atoms, in a systematic fashion. We discuss a number of recent algorithmic advances that enable these studies.

Tuesday, August 30, Session 7: 1:50-2:25
First Principles III
Adaptively Compressed Exchange Operator
Lin Lin, *University of California, Berkeley*

The Fock exchange operator plays a central role in modern quantum chemistry, such as in Hartree-Fock calculations and Kohn-Sham density functional theory calculations with hybrid exchange-correlation functionals. The Fock exchange operator significantly increases the computational cost for solving the associated Kohn-Sham eigenvalue problem. We develop the adaptively compressed exchange operator formulation, which greatly reduces the computational cost associated with the Fock exchange operator without loss of accuracy. The ACE formulation does not depend on the size of the band gap, and thus can be applied to insulating, semiconducting as well as metallic systems. Numerical results indicate that the ACE formulation can become advantageous even for small systems with tens of atoms.

Tuesday, August 30, Session 8: 3:00-3:35
Coarse-Grained Atomistics
Speculatively Parallelized Temperature Accelerated Dynamics
Arthur Voter, Richard Zamora, Danny Perez, *Los Alamos National Laboratory*

Temperature accelerated dynamics (TAD) is a powerful atomistic approach for reaching long time scales for systems whose dynamics are characterized by activated processes, especially when the energy barriers are high. In TAD, a basin-confined simulation at a high temperature is employed to discover attempted escape events in a way that allows the assignment of a time t_low (approximate, but controllably accurate) for the same event occurring in a hypothetical trajectory at the lower, proper temperature. High- and low-temperature escape times typically will not occur in the same order, as high-barrier processes are sped up more by the increase in temperature. After the basin-confined, high-temperature trajectory has reached a certain total time (t_stop), one can say with a specified confidence that the first escape event at low temperature has been observed. The system is then moved to the new state corresponding to this event, the clock is advanced by t_low for this event, and the TAD procedure is begun again in the new state. In this talk, I will describe a novel approach for parallelizing TAD: speculatively parallelized TAD (SpecTAD) [1]. In SpecTAD, wespawn a child process in parallel each time an attempted escape event is observed, if it has a chance of becoming the accepted event. This child process, which corresponds to a complete, independent TAD simulation in the state to which the system made its attempted escape, is continued until and unless it becomes clear that this event is not the one that will be accepted by the parent TAD simulation. SpecTAD gives a significant additional speedup over conventional TAD when t_stop is much longer than the time at which the ultimately accepted event is first attempted. A SpecTAD trajectory can advance from state to state as rapidly as the (correct) transitions occur at high temperature. Moreover, this approach can be combined efficiently with the use of parallel replica dynamics to accumulate the high-temperature time more quickly. I will describe the SpecTAD method, give examples of its application, and discuss situations where its ability to eliminate the waiting time until t_stop introduces new possibilities for simulations that would be unfeasible with conventional TAD. [1] R.J. Zamora, B.P. Uberuaga, D. Perez, and A.F. Voter, The modern temperature-accelerated dynamics approach. The Annual Review of Chemical and Biomolecular Engineering 7, 3.1-3.24, (2016).

Tuesday, August 30, Session 8: 3:35-4:10
Coarse-Grained Atomistics
Accelerated Multiscale Simulation of Nanoindentation Using Hyper-Quasicontinuum Method
Woo Kyun Kim, *University of Cincinnati*

Over the past decades atomistic simulations such as molecular dynamics (MD) have made significant contributions to modeling materials by providing direct access to atomic-scale mechanisms which cannot be observed experimentally. Furthermore, atomistic simulations have been indispensable in developing predictive models for material properties and responses based on the fundamental understanding of atomic-level processes. However, even with the aid of high-performance computing available today, the length and time scales of systems that can be modeled by atomistic simulations are by several orders of magnitude different from those of macroscopic systems of technological interest. Recently, Kim and Tadmor with their coworkers have developed a novel multiscale method, called hyper-QC, which can extend both length and time scales simultaneously. Hyper-QC combines quasicontinuum (QC), a spatial multiscale method, and hyperdynamics, an accelerated MD scheme, on a single platform. In this talk, the hyper-QC simulation results of nanoindentation of crystalline materials will be presented. Nanoindentation is the small-length scale counterpart to the conventional indentation test on macroscopic length scales used to measure hardness and the deformation mechanisms in nanoindentation tests have not been completely understood. Moreover, due to the short time scale problem, most MD simulations have been performed at indentation rates that are many orders of magnitude larger than those used in actual experiments. Hyper-QC enables the simulation at the indentation rates up to three orders of magnitude lower than that of the conventional MD scheme. Finally, a novel bias potential for hyperdynamics using the slip mechanism of crystals will be introduced, which is computationally less expensive than the originally proposed bias potential using the eigenvalue/eigenvector of the Hessian.

Tuesday, August 30, Session 8: 4:10-4:50
Coarse-Grained Atomistics
Coarse-Grained Modeling of Nanoconfinement in Structural Nanocomposites
Sinan Keten, *Northwestern University*

Natural and engineered structural (load-bearing) nanocomposites often try to exploit microphases that are confined in nanoscale dimensions to achieve remarkable mechanical properties. However, the emergent performance of these materials depends strongly on both the chemistry of the interfaces and the microstructure of the material system, which complicates their design. In this talk, I will present a new computational materials-by-design paradigm for understanding phenomena occurring at such disparate scales. I will discuss several cases where the coupling between nanostructure and chemical structure will lead to intriguing phenomena, such as polymers with more or less identical bulk properties exhibiting contrasting behavior under nanoconfinement in thin films. Drawing an analogy between thin films and nanocomposites, I will illustrate how understanding thin film simulations help us design better load-bearing nanocomposites with nanocellulosic fillers.

Wednesday, August 31, Session 9: 8:30-9:05
Scale-Bridging Methods
Bridging Timescales: Automating Diffusivity Calculations for Interstitial and Solute Diffusion from First-Principles
Dallas R. Trinkle, *University of Illinois, Urbana-Champaign*

Mass transport controls crucial materials processing, such as segregation and precipitation, and properties, such as ionic conductivity, in a wide variety of materials. First-principles methods can determine the activated state energies at the atomic level involved in mass-transport such as vacancies moving in a crystal. Upscaling from activation barriers to mesoscale mobilities requires the solution of the master equation for diffusivity. For all but the simplest cases of interstitial diffusivity, and particular approximations with vacancy-mediated diffusion on simple lattices, calculating diffusivity directly is a challenge. This leaves two choices: uncontrolled approximations to map the problem onto a simpler (solved) problem, or a

stochastic method like kinetic Monte Carlo, which can be difficult to converge for cases of strong correlations. Moreover, without analytic or semi-analytic solutions, evaluating derivatives of transport coefficients is also difficult. We describe and demonstrate the development of direct and automated Green's function solutions for transport that take full advantage of crystal symmetry. We apply this to a variety of problems, from interstitial diffusivity of light elements in magnesium-including the elastodiffusion tensor and activation volume tensor---to vacancy mediated diffusion of substitutional solutes in magnesium, all of which include correlation effects on transport. The underlying automation also makes the extension of first-principles transport databases significantly more practical and reduce uncontrolled approximations.

Wednesday, August 31, Session 9: 9:05-9:40
Scale-Bridging Methods
Multiscale Simulations of Wave Propagation in Heterogenous Media
Celia Reina, Chenchen Liu, *University of Pennsylvania*

This talk will discuss a new variational coarse-graining framework for heterogeneous media, in the spirit of computational homogenization methods (FE2), that allows for a seamless transition from the traditional static scenario to the dynamic case. The method is based on an extension of the traditional Hill averaging relations that allow for a micro-macro coupling in the presence of microinertia (with or without body forces), general material behavior as well as discrete or continuous representations of the material and its deformation. The method will be successfully illustrated over a one-dimensional layered composite, where the dispersion properties are accurately predicted.

Wednesday, August 31, Session 9: 9:40-10:15
Scale-Bridging Methods
Multiscale Computation for Materials Modeling
Jaroslaw Knap, Kenneth W. Leiter, Brian C. Barnes, Richard Becker, Adam Sokolow, Joshua C. Crone, Oleg Borodin, *Army Research Laboratory*

Over the last few decades, multi-scale modeling (MSM) has become a dominant paradigm in materials modeling and simulation. The practical impact of MSM depends, to a great extent, on its ability to utilize modern computing platforms. However, since there are no general numerical and computational frameworks for MSM, the vast majority of multi-scale material models or simulations are developed on a case-by-case basis. We seek to formulate an adaptive computational framework for MSM. We do not plan to develop a specific method for MSM simulations, but instead, aim to develop a broad and flexible computational framework for designing and developing such simulations. Our focus is primarily on new scalable numerical algorithms applicable to a wide range of MSM applications and, more specifically, to scale-bridging. These algorithms fall into one of the three areas: i) adaptive computational strategies for MSM, ii) algorithms for scale-bridging in MSM, and iii) algorithms for development of surrogate models to reduce the computational cost associated with MSM. First, we present a formulation of our computational MSM framework. Subsequently, we describe development of a two-scale multi-scale model of an energetic material, as well as, a high-throughput capability for battery research, both utilizing our framework.

Wednesday, August 31, Session 10: 10:35-11:10
Metal Plasticity
Strain Rate, Grain Size Distribution and Avalanche Behavior in Nanocrystaline Metals
Marisol Koslowski, Lei Cao, *Purdue University*

Dislocation dynamics simulations have advanced the understanding of the mechanical behavior of polycrystalline materials. However, the results of these simulations are limited by the lack of advanced models that include complex mechanisms such as grain boundary deformation and dissociation into partials as well as realistic representations of texture and grain structure.

The deformation of ultra-fine and nanocrystalline metals with a phase-field approach to dislocation dynamics. Grain-boundary mediated deformation and the gamma surface calculated directly from atomistic simulations in several fcc materials are included with different grain

configurations, initial dislocation densities, grain boundary energetics and strain rates. The simulations predict the following results: i) the yield stress depends not only on the average grain size but also on the grain size distribution and the grain boundary energy ii) configurations with smaller average grain size have a larger density of partial dislocations but in agreement with in situ X-ray experiments show no increase of the stacking fault density in nanocrystalline nickel; iii) the ratio between partial and full extended dislocation densities varies with the applied strain and strain rate, suggesting that there is no well-defined transition from full dislocation to partial dislocation-mediated plasticity that is based only on the grain size; iv) there is a transition from continuum plastic flow to avalanche behavior that depends on the strain rate and the average grain size.

Wednesday, August 31, Session 10: 11:10-11:45
Metal Plasticity
Predicting the Temperature Dependence of the Yield Strength in BCC Metals using Atomistically-Informed Crystal Plasticity Calculations

Jaime Marian[1], David Cereceda[2], Martin Diehl[3], Franz Roters[3], Dierk Raabe[3]
[1]Univeristy of California Los Angeles, [2]Johns Hopkins University, [3]Max-Planck-Institut für Eisenforschung

The plastic behavior of BCC single crystals is governed by screw dislocation glide on close-packed crystallographic planes. Screw dislocation motion occurs via thermally-activated nucleation and relaxation of so-called kink pairs on a periodic energy substrate known as the Peierls potential. A long standing puzzle regarding BCC plasticity has been the discrepancy between the measured values of the yield and flow stress in tensile deformation tests and the calculated values of the Peierls stress at the atomistic scale. Here, we present a model that unifies both concepts and provides a justification for the differences in terms of the non-Schmid behavior displayed by BCC crystals. Our model consists of a crystal plasticity microstructural engine parameterized entirely using atomistic calculations, that includes full non-Schmid effects as well as a physically-consistent flow rule constructed on the basis of thermally activated screw dislocation glide. We apply the methodology to yielding in tungsten and show that available experimental measurements can be explained and reproduced by accounting for these two very important features of BCC plasticity. The validated methodology is used to predict the strength as a function of several state variables in W single crystals.

Wednesday, August 31, Session 10: 11:45-12:20
Metal Plasticity
Decohesion Relationships for Grain Boundary Fracture in Nickel Extracted from Molecular Dynamics Simulations

Douglas Spearot[1], Doruk Aksoy[1], Wesley Barrows[2], Remi Dingreville[3]
[1]University of Florida, [2]University of Arkansas, [3]Sandia National Laboratories

In molecular dynamics (MD) studies of the mechanical properties of grain boundaries, it is common for a range of grain boundary structures to be sampled by incrementing the misorientation angle of the grain boundary around a fixed misorientation axis. The limitation of this approach is that as the misorientation angle of the grain boundary is rotated, the stress-strain response and the fracture behavior of the grain boundary become a convolution of the orientation dependent lattice properties and interface structure. To isolate the influence of grain boundary structure on intergranular fracture, this work presents a different approach to select grain boundaries for atomistic analysis. Specifically, sets of grain boundaries will be analyzed whose lattice orientations transverse isocurves within a stereographic triangle associated with critical lattice properties (e.g., elastic stiffness, primary Schmid factor). This provides a route to deconvolute the role of the grain boundary structure on decohesion from the influence of the surrounding lattices. This approach is used to study decohesion of equilibrium Ni grain boundaries and Ni grain boundaries with segregated H. Decohesion behavior is assessed through extraction of traction-separation relationships, employing atomistic cohesive zone

volume elements (CZVEs). Results show that increasing hydrogen coverage can asymmetrically influence crack tip velocity during steady-state crack propagation, and generally leads to a decrease in the work of separation and peak strength.

Wednesday, August 31, Session 11: 1:30-2:05
Mechanics of Materials
Intrinsic Scale Effects in Metal Deformation

Christopher Woodward[1], Satish Rao[2], Ahmed Hussein[1], Brahim Akdim[1], Edwin Antillon[1], Dennis Dimiduk[3]
[1]Air Force Research Laboratory, [2]École Polytechnique Fédérale, [3]Blue Quartz Software

Transition in deformation behavior in samples across the macro-nano scales can be used to inform size dependent plasticity methods. Scale effects can be quantified and validated using lower scale, physics-based models. Recent experiments have shown strong size effects in metal micro-pillars with dimensions below ~100 micro-meters. This size dependent behavior is consistent with deformation occurring below a characteristic dislocation correlation length. Micro-scale dislocation evolution simulations exhibit the same behavior and reveal the mechanistic source of strengthening (and stochastic flow) at theses scales. In this work, large scale atomistic and dislocation dynamics simulations are used to assess the aspects of ensemble hardening in simple metals. Atomistic simulations illustrate the effects of cross slip on full 3-d simulations of forest hardening. The work hardening rates of micro pillars, uniaxial loaded along <100>, <110>, and <111>, are calculated using dislocation dynamics simulations. Simulations include dislocation intersection cross slip which enhances the rapid increase in dislocation density. Analyses of the evolving dislocation ensembles, including the formation of strong dislocation heterogeneities are reviewed.

Wednesday, August 31, Session 11: 2:05-2:40
Mechanics of Materials
Resolving the Correlation between Microstructure and Nanoscale Deformation Mechanisms in Metallic Nanostructured Materials

Garritt J. Tucker, *Drexel University*

As atomistic modeling methods have pursued a more complete understanding of the structure and deformation of metallic microstructures, two outstanding issues have remained: developing (1) more realistic microstructures and (2) metrics to quantify the operative mechanisms. This research leverages atomistic studies of the mechanical deformation of nanocrystalline metals to illustrate how more meaningful correlations can be extracted from simulations using new methods for generating more realistic microstructures and continuum-based metrics for post-simulation analysis. This research highlights the utility of calculating both deformation and rotation fields within the nanostructures to resolve the activity and role of various nanoscale deformation mechanisms, such as dislocations, interfaces, and twin boundaries in accommodating strain within the microstructure. By leveraging these metrics, the competition between mechanisms can be quantified and strain maps demonstrate how microstructural variables influence accommodation at the nanoscale, including twinning. The effect of differences in the initial microstructure, such as grain shape and grain boundary structure, on the active strain accommodation mechanisms is provided. Finally, this research shows how dominant deformation modes can vary due to grain size, composition, and microstructural topology in metallic alloys, and suggests avenues for multiscale modeling.